II. Claims 22-29, drawn to a method [of] searching [a] database of molecules for molecules that are similar to a target molecule by a method of determining a shape space of a set of molecules, classified in Class 707, subclass 100.

III. Claims 30-48, drawn to a mathematical method of constructing an ellipsoidal gaussian representation of a molecule field, classified in Class 703, subclass 2.

IV. Claims 49-56, drawn to a method of associating a first atom in a first molecule with an atom in a second molecule, classified in Class 703, subclass 12.

V. Claims 57-68, drawn to a method of searching database for at least one part of a molecule that is similar to at least one part of a target molecule structure, classified in Class 707, subclass 100.

VI. Claims 69-78, drawn to a method of organizing a database via stored median, T, distances of N objects for facilitating searching the database, classified in Class 707, subclass 101.

VII. Claims 79-96, drawn to a method of organizing database via minimal distance stored for K key objects in a database of N objects for facilitating searching the database, classified in Class 707, subclass 101.

VIII. Claims 97-102, drawn to a mathematical method of constructing a pseudo-surface of an ellipsoidal gaussian representation[s] of a molecular field, classified in Class 703, subclass 2.

IX. Claims 103-130, drawn to a method of constructing at least one single ellipsoidal gaussian function representation for a vacant space, classified in Class 703, subclass 2.

X. Claims 131-136, drawn to a method of predicting the biological activity of a molecule of interest via [a] statistical method, classified in Class 703, subclass 11.

XI. Claim 137, drawn to a method of identifying a fragment of a molecule, classified in Class 702, subclass 29.

XII. Claims 138 and 139, drawn to a method of assessing the diversity of a set of molecules stored in a database on a computer, classified in Class 702, subclass 23.

The Examiner has further indicated that an election of any of Groups I, II, VI and VII must be accompanied by an election of one of the following species:

A a molecular field;
B a steric field of a molecule;
C an electrostatic potential around a molecule;
D a gaussian molecular field.

Applicants hereby provisionally elect the subject matter of **Group II**, claims 22-29, drawn to a method of determining a shape space of a set of molecules and searching a database of molecules for molecules that are similar to a target molecule.

Applicants further provisionally elect **Specie A**, a "molecular field" and indicate that claims 22, 27-29 read upon specie A.

Applicants respectfully request that the above-made remarks be made of record in the file history of the present application. Applicants retain the right to petition from the restriction requirement under 37 C.F.R. § 1.144.

No fee is believed due with this response. However, should the Commissioner determine otherwise, he is hereby authorized to charge any fees associated with filing this Response to Pennie & Edmonds Deposit Account No. 16-1150. A copy of this sheet is enclosed.

Respectfully submitted,

Date June 10, 2002

Richard G.A. Bone (Reg. No.)
Limited Recognition Under 37 C.F.R. § 10.9(b)
(Copy of Certificate Enclosed)

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